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RESEARCH REPORT No. CX-34

The Application of the Impulse Approximation to the Inelastic Scattering of Electrons by Hydrogen Atoms

RICHARD AKERIB and SIDNEY BOROWITZ

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Abstract

A calculation of the ionization cross section and the excitation cross section to the 2S and 2P states of hydrogen by collision with electrons is carried through, using an impulse approximation. The results are then compared to the experimental results when available and to the various theoretical calculations. The cross sections obtained compare favorably with experiment except for the excitation to the 2S state. The calculations carried out by these methods are considerably simpler than the usual approximation methods, and the agreement of the results with experiment indicates that it is a simpler and better method to use for the computation of cross sections in the scattering of electrons by atoms.

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1. Introduction

The problem of the scattering of electrons by atoms is of theoretical interest since it serves as a model for other many-body scattering processes and since, in this case, the law of force between the particles involved is known. There is also a practical motivation in this problem. Whenever one considers the passage of an electron through a cloud chamber, the propagation of electromagnetic radiation through the ionosphere or gaseous discharges, the scattering of electrons by atoms plays a predominant role. Inelastic processes play an important role whenever, in a physical process, an electron transfers part of its energy to the internal degrees of freedom of the scattered system. The purpose of this paper is to apply an approximation method, hitherto unused in this field, to the analysis of this problem.

We shall be dealing in this paper with the ionization of atomic hydrogen and the excitation of a hydrogen atom from its ground state to the $n = 2$ level due to a collision with an electron. Our interest in hydrogen is two-fold. Atomic hydrogen is one of the basic constituents of the universe, and thus the problem has an intrinsic interest of its own. Beyond this, the scattering of electrons by hydrogen can be used as a model for approximation techniques which can possibly be generalized to deal with more complex situations. In recent years, experimental techniques have improved so much that one is able to carry out experiments involving atomic hydrogen and analyze the results to separate the various inelastic processes. For example,Fite in the United States and Boyd and Green in England have been able to investigate the ionization and excitation of hydrogen by electron impact. In addition to yielding data with regard to the elementary processes involved, the results serve as a test for the various approximation methods used for the analysis of the inelastic scattering of electrons by hydrogen atoms.

The approximations that have been used to date are the Born approximation, the distorted wave method and some variational techniques. The problem involved in an approximation method is to find a reasonable description of the wave function of the electron-hydrogen system. In the Born approximation, one assumes that the interaction between the electron and the hydrogen atom is so small that one can choose for the total wave function the product of a plane wave for the incident electron and a wave function describing the unperturbed atomic system. In the distorted wave approximation, one tries to make an estimate of the distortion of the incident wave by the atomic system. In using variational methods, one calculates some expression describing the scattering process which is stationary with respect to the choice of the unknown wave function of the system: that is, one hopes that an error of order ϵ in the wave function will result in an error of order ϵ^2 in the description of the scattering process.

A comparison of the experimental results with the theoretical results shows that the Born approximation tends to overestimate by a considerable amount the value of the cross section at low energies. In general, the maximum of the calculated cross section occurs at a value of the energy less than the value at which the actual experimental maximum occurs. Even the second Born approximation gives a value which is still too large for the cross section, although it is closer.

In this paper, we have calculated the inelastic cross section to the $n = 2$ level and the ionization cross section of hydrogen for collisions with electrons using the 'Impulse Approximation' developed by G. Chew[1]. The basic idea of this approximation is to consider the target particles as frozen during the collision - that is, to disregard the fact that the atomic particles are bound rather than free. If the cross section for a collision between two particles is known, as it is in this case, then one can calculate the cross section due to the two two-body collisions. To take into account the fact that the two target particles are bound, one averages over the charge distribution of the bound particles in the initial and final states. In order to account for the assumption that the bound particles do not interact, one replaces the charge distribution with an equivalent momentum distribution.

The validity of this approximation can be seen, from physical considerations, to involve the transit time of the incident particle across the target system and the period of the bound particle. To estimate the circumstances under which this approximation is valid for the scattering of electrons by hydrogen atoms, one proceeds in the following way. The radius of the hydrogen atom in the ground state is a_o. If the orbital velocity of the bound electron is v_2, then the period of the electron is

$$t_2 \approx 2\pi a_o/v_2 .$$

If v_1 is the velocity of the incident electron, then the time of transit is

$$t_1 = 2a_o/v_1 .$$

The validity of the impulse approximation depends on

$$t_1 \ll t_2$$

or

$$v_2/v_1 \ll \pi .$$

At threshold, $v_1 = v_2$ and thus, as one approaches threshold, the results may not be too reliable. As v_1 increases, v_2/v_1 decreases so that for an incident energy of 100 e.v. $v_2/v_1 = 1/3$. Hence, as the incident energy increases the approximation should yield results that compare more favorably with experiment.

This paper is divided in the following way: a review of the various approximation methods is taken up in Section 2. In Section 3, we derive the fundamental formulas of the Impulse Approximation and state these for ionization and excitation. Section 4 deals with the ionization cross section while Sections 5 and 6 deal respectively with the cross sections for the 2S and 2P states. Section 7 summarizes the results. The evaluation of the various integrals occurring in the body of the work is done in Appendices A, B and C.

2. Review of former work

The problem of the scattering of an electron by a hydrogen atom can be found as a solution of the following Schrödinger equation with appropriate boundary conditions:

$$(1)\quad \left\{ -\frac{\hbar^2}{2m}(\Delta_1 + \Delta_2) - \frac{e^2}{r_1} - \frac{e^2}{r_2} + \frac{e^2}{r_{12}} \right\} \Psi(\vec{r}_1,\vec{r}_2) = E\,\Psi(\vec{r}_1,\vec{r}_2).$$

In the above equation, the center of mass of the system is located at the proton which is assumed to have an infinite mass; $\vec{r}_1$ and $\vec{r}_2$ are the coordinates of the incident and bound electrons, respectively, and E is the total energy of the system. The equation is not separable because of the term e^2/r_{12}. We shall now discuss the boundary conditions to be imposed on the solution of (1) and the information which is needed from the solution.

Later we shall discuss the various approximations that have been used.

We desire a solution of (1) which has the asymptotic form

$$\Psi(\vec{r}_1,\vec{r}_2) \underset{r_1 \to \infty}{\sim} \Phi_0(\vec{r}_2)e^{i\vec{k}_0\cdot\vec{r}_1} + \sum \Phi_n(\vec{r}_2)\,\frac{e^{ik_n r_1}}{r_1}\,f_n(\theta_1,\phi_1) \tag{2}$$

where

$$k_n^2 = k_0^2 - \frac{2m}{\hbar^2}(E_n - E_0) \tag{2a}$$

and $\Phi_n(\vec{r}_2)$ are the hydrogenic wave functions. The summation includes integration over the continuum states. $f_n(\theta_1,\phi_1)$ is the scattered amplitude for excitation to the nth state. It is related to the differential cross section for direct scattering by the relation

$$\sigma_{nd}(\theta,\phi)d\,\omega = \frac{k_n}{k_0}\,|f_n(\theta,\phi)|^2 d\,\omega. \tag{3}$$

Instead of taking the limit as $r_1 \to \infty$, we can allow r_2 to approach ∞. This will describe the process wherein the incident electron exchanges roles with the bound electron. The asymptotic form of the wave function in this case is

$$\Psi(\vec{r}_1,\vec{r}_2) \underset{r_2 \to \infty}{\sim} \sum_n g_n(\theta_2,\phi_2)\Phi_n(r_1)\,\frac{e^{ik_n r_2}}{r_2} \tag{4}$$

where $g_n(\theta_2,\phi_2)$ is the exchange scattered amplitude and is related to the exchange differential cross section by

$$\sigma_{ne}(\theta,\phi)\,d\,\omega = \frac{k_n}{k_0}\,|g_n(\theta,\phi)|^2 d\omega \quad . \tag{5}$$

The differential scattering cross section for the process is a combination of direct and exchange scattered amplitudes. One must also take into account the spins of the two electrons. This leads to

$$\sigma_n \, d\omega = \frac{k_n}{k_o} \left\{ \frac{1}{4} \, |f_n + g_n|^2 + \frac{3}{4} \, |f_n - g_n|^2 \right\} . \tag{6}$$

Let us now derive the general relations upon which most of these approximations are based. To this end, we expand $\Psi(\vec{r}_1, \vec{r}_2)$ in terms of the complete set of hydrogenic wave functions $\Phi_n(\vec{r}_2)$

$$\Psi(\vec{r}_1, \vec{r}_2) = \sum \Phi_n(\vec{r}_2) F_n(\vec{r}_1). \tag{7}$$

As usual, the summation sign includes an integral over the continuum states of hydrogen. Substitution of (7) into (1) leads to

$$\sum \Phi_n(\vec{r}_2) \left\{ \Delta_1 + k_n^2 \right\} F_n(\vec{r}_1) = \frac{2me^2}{\hbar^2} \left\{ \frac{1}{r_{12}} - \frac{1}{r_1} \right\} \Psi(\vec{r}_1, \vec{r}_2) \tag{8}$$

where we have used the Schrödinger equation for the hydrogen atom satisfied by $\Phi_n(\vec{r}_2)$. We multiply both sides of (8) by $\Phi_m(\vec{r}_2)$ and integrate over $\vec{r}_2$. In making use of the orthogonality of the hydrogenic wave functions, we obtain:

$$\left\{ \Delta_1 + k_n^2 \right\} F_n(\vec{r}_1) = \sum U_{nm}(\vec{r}_1) F_m(\vec{r}_1) \qquad (n = 0, 1, 2, \ldots) \tag{9}$$

where

$$U_{nm} = \frac{2me^2}{\hbar^2} \int d\vec{r}_2 \, \Phi_n^*(\vec{r}_2) \left\{ \frac{1}{r_{12}} - \frac{1}{r_1} \right\} \Phi_m(\vec{r}_2). \tag{10}$$

For exchange scattering, we expand $\Psi(\vec{r}_1, \vec{r}_2)$ in terms of the complete set of hydrogenic wave functions $\Phi_n(\vec{r}_1)$

$$\Psi_n(\vec{r}_1,\vec{r}_2) = \sum G_n(\vec{r}_2)\, \Phi_n(\vec{r}_1). \tag{11}$$

Application of the same method used to derive (9) leads to

$$(\Delta_2 + k_n^2)\, G(\vec{r}_2) = \frac{2me^2}{\hbar^2} \int d\vec{r}_1\, \Phi_n^*(\vec{r}_1)\left(\frac{1}{r_{12}} - \frac{1}{r_2}\right) \Psi(\vec{r}_1,\vec{r}_2)\ . \tag{12}$$

Each of equations (9) and (12) consists of an infinite number of coupled integro-differential equations and cannot be solved exactly. They are solved approximately by using various schemes. We shall look into these briefly.

A. Born approximation

Let us first consider (9). The Born approximation is obtained by assuming that all the terms on the right-hand side of (9) are negligible except for the term associated with the incident wave. This is equivalent to assuming that the perturbation due to the interaction between the two electrons is small. Equations (9) take the form:

$$(\Delta_1 + k_n^2)\, F_n(\vec{r}_1) = U_{no}\, e^{i\vec{k}_o\cdot\vec{r}_1} \quad . \tag{13}$$

To solve this equation, we use Green's function for the operator $\Delta_1 + k_n^2$ satisfying the appropriate boundary conditions. This yields

$$F_n(\vec{r}_1) = -\frac{1}{4\pi} \int U_{no}(\vec{r}_1)\, e^{i\vec{k}_o\cdot\vec{r}_1}\, \frac{e^{ik_n|\vec{r}_1 - \vec{r}_1'|}}{|\vec{r}_1 - \vec{r}_1'|}\, d\vec{r}_1' \ . \tag{14}$$

If we now take the limit as $\vec{r}_1 \longrightarrow \infty$, we obtain

$$F_n(\vec{r}_1) \underset{r_1}{\sim}> \infty\ f_n(\theta,\phi)\, \frac{e^{ik_n r_1}}{r_1} \tag{15}$$

with

$$(16) \qquad f_n(\theta,\phi) = -\frac{1}{4\pi} \int U_{no}(r_1) e^{i(\vec{k}_o - \vec{k}_n)\cdot\vec{r}_1} \, d\vec{r}_1 \quad .$$

For ionization, (16) takes the form:

$$(17) \qquad f_\kappa(\theta,\phi) = -\frac{1}{4\pi} \frac{2me^2}{\hbar^2} \int d\vec{r}_1 d\vec{r}_2 \, e^{-i\vec{k}_\kappa \vec{r}_1} \, \Phi^*_\kappa(\vec{r}_2)\left(\frac{1}{r_{12}} - \frac{1}{r_2}\right) e^{i\vec{k}_o \cdot \vec{r}_1} \, \Phi_o(\vec{r}_2).$$

In equation (17) $\Phi_\kappa(\vec{r}_2)$ is the wave function of an electron of momentum in the continuum field of the proton. Mott and Massey[2] use the expression

$$(18) \qquad \Phi_\kappa(\vec{r}_2) = \frac{\kappa}{2\pi} \left\{ \frac{n}{1-e^{-2\pi n}} \right\}^{1/2} \frac{e^{i\kappa r_2}}{\Gamma(1-in)} \int_0^\infty du \, u^{-in} e^{-u} J_o(2\sqrt{i\kappa \xi u}\,)$$

where

$$\xi = r(1+\cos\Theta) \qquad\qquad n = 1/\kappa a_o \ .$$

$$\cos\Theta = \cos\theta_1 \cos\theta_2 + \sin\theta_1 \sin\theta_2 \cos(\theta_1 - \phi_2)$$

and $J_o(2\sqrt{i\kappa \xi u}\,)$ is the Bessel function of zero order and $\Gamma(1-in)$ is the gamma function. If we substitute (18) into (17) and integrate over $\vec{r}_1$ and $\vec{r}_2$, we obtain for the differential scattering cross-section

$$I_\kappa(\theta,\phi)\,d\omega d\kappa = \frac{2^{10}\kappa k_\kappa}{a_o^2 \, kK^2} \, \frac{\mu^6\left\{K^2 + \frac{1}{3}(\mu^2 + \kappa^2)\right\}}{1 - \exp(-2\pi\mu/\kappa)}$$

$$(19) \qquad \times \frac{\exp\left\{-\frac{2\mu}{\kappa}\tan^{-1}\left(2\mu\kappa/\left[K^2 - \kappa^2 + \mu^2\right]\right)\right\}}{\left\{\mu^4 + 2\mu^2(K^2 + \kappa^2) + (K^2 - \kappa^2)^2\right\}^3} \, d\omega d\kappa$$

where integration over all angles of ejection of the bound electron has been carried out. In (19) κ is the wave number of the ejected electron

$$\mu = Z = 1/a_o$$

$$K^2 = (k^2 + \kappa^2 - 2k\kappa\cos\theta).$$

This expression was integrated numerically by W. Fite[3]. The curve obtained is plotted in Figure 1. Note that at high energies, the value of the total cross section is too high.

For the excitation to the state n from the state m by electron impact, Mott and Massey[4] give the expression for direct scattering

$$I_{mn}(K)dK = \frac{4\pi}{a_o^2 k^2} \frac{dK}{K^3} |\epsilon_{mn}(K)|^2 \tag{20}$$

where

$$\epsilon_{mn} = \int e^{i\vec{K}\cdot\vec{r}}\, \Psi_m \Psi_n^* \, d\vec{r} \,. \tag{21}$$

For excitation from the ground state to the state $(n\ell m)$ they give:

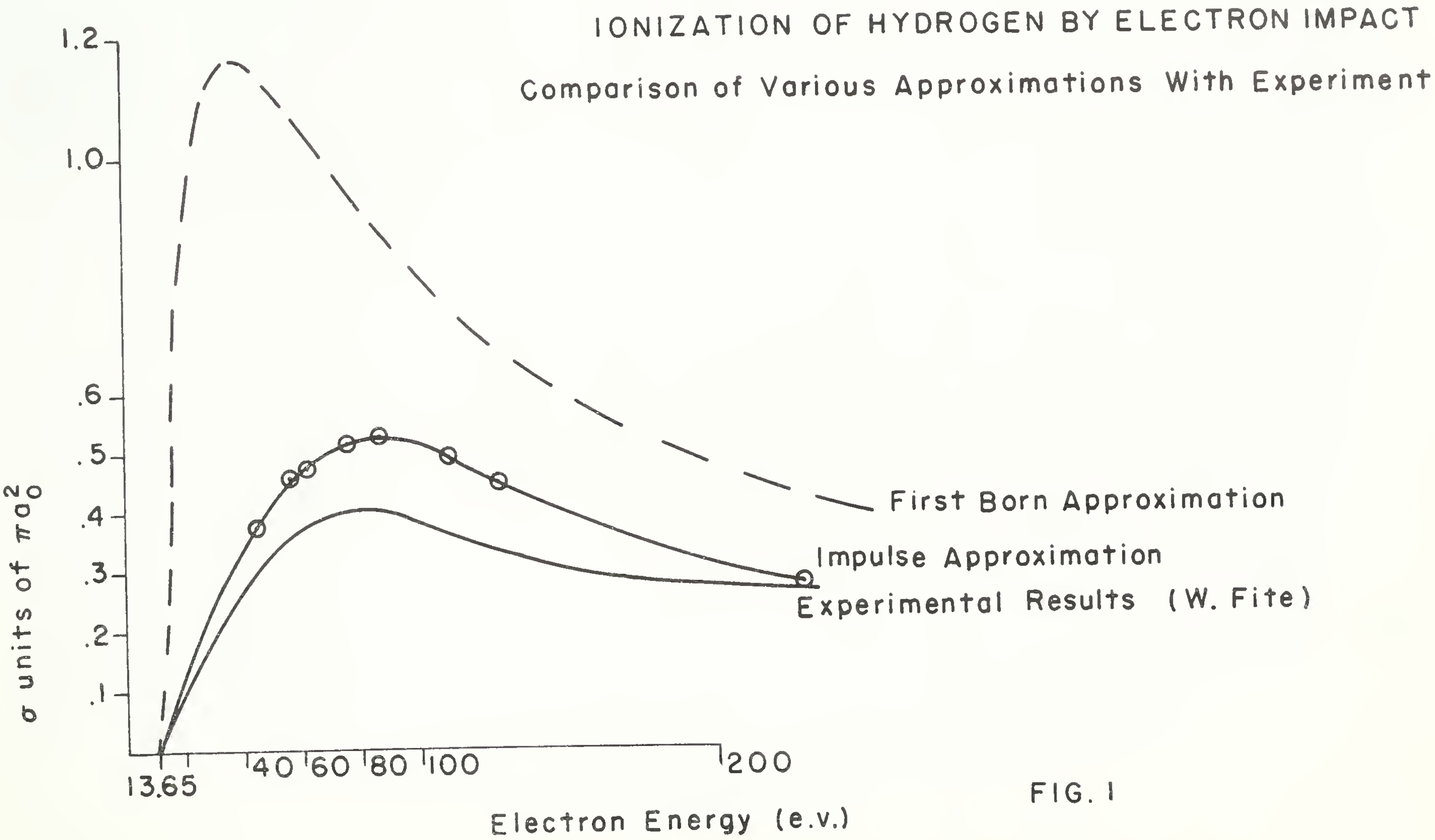
$$\begin{aligned} \epsilon_{n\ell m} = {} & 2^{2\ell+3} n^{\ell+1} (2\ell+1)^{1/2} (\ell+1)! \left[\frac{(n-\ell-1)!}{(n+\ell)!}\right]^{1/2} (Ka_o)^\ell \\ & \times \frac{\{(n-1)^2+4\zeta^2\}^{1/2(n-\ell-3)}}{\{(n+1)^2+4\zeta^2\}^{1/2(n+\ell+3)}} \left[(n+1)\left\{(n-1)^2+4\zeta^2\right\} C^{\ell+2}_{n-\ell-1}(x) \right. \\ & - 2n\left\{(n-1)^2+4\zeta^2\right\}^{1/2}\left\{(n+1)^2+4\zeta^2\right\}^{1/2} C^{\ell+2}_{n-\ell-2}(x) \\ & \left. + (n-1)\left\{(n+1)^2+4\zeta^2\right\} C^{\ell+2}_{n-\ell-3}(x)\right] \end{aligned} \tag{22a}$$

where

$$x = (n^2-1+4\zeta^2)\left[\left\{(n+1)^2+4\zeta^2\right\}\left\{(n-1)^2+4\zeta^2\right\}\right]^{-1/2} \tag{22b}$$

$$\zeta = \frac{1}{2} Ka_o \tag{22c}$$

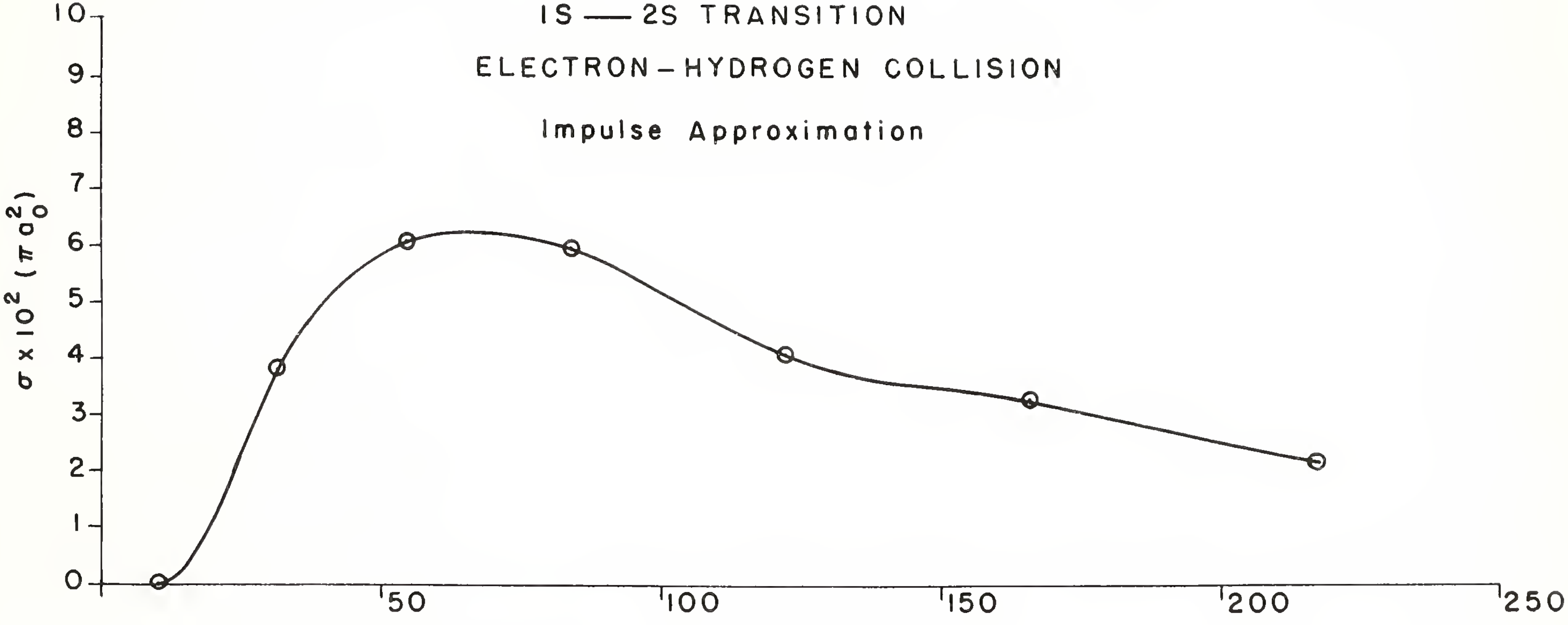
and $C_s^\nu(x)$ are the Gegenbauer polynomials. The curves obtained for the total cross section for excitation to the 2S and 2P from the ground state are plotted respectively in Figures 2 and 3. Again the values are too high.



IONIZATION OF HYDROGEN BY ELECTRON IMPACT

Comparison of Various Approximations With Experiment

FIG. 1

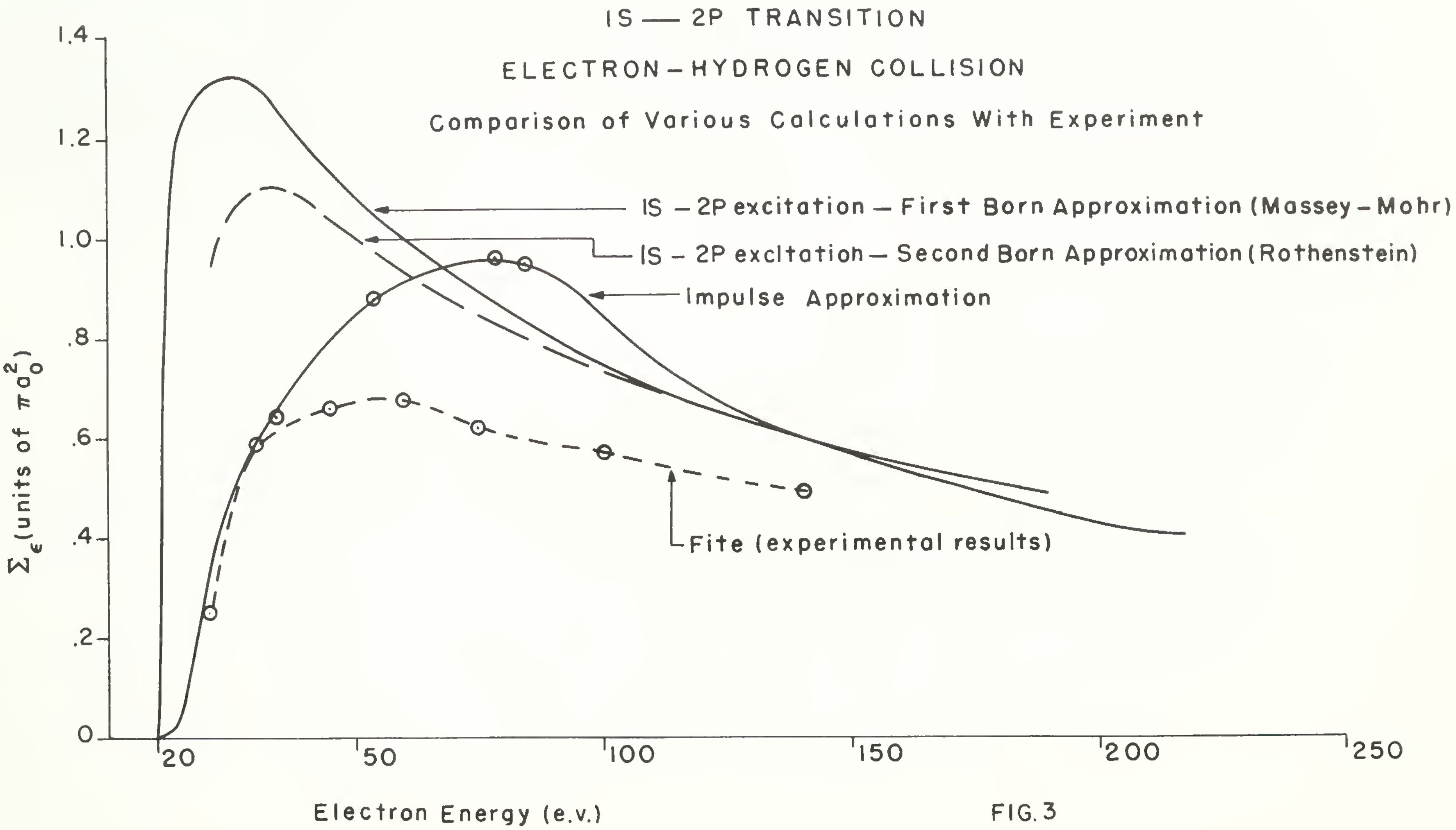


IS —— 2S TRANSITION

ELECTRON – HYDROGEN COLLISION

Impulse Approximation

FIG. 2


IS —— 2P TRANSITION

ELECTRON – HYDROGEN COLLISION

Comparison of Various Calculations With Experiment

FIG. 3

Rothenstein[5] has carried out the second Born approximation for excitation to the 2P state. Although the values are better at intermediate energies, they are still not in good agreement with experiment. These results are plotted in Figure 3.

B. Distorted wave approximation

In this method, one assumes that all the non-diagonal elements of the matrix U_{nm} given in (9) are small except for the ones associated with the incident wave. No assumptions are made regarding the diagonal elements. Thus (8) reduces to

$$(23a) \qquad (\Delta_1 + k_o^2 - U_{oo})F_o(\vec{r}_1) = 0$$

$$(23b) \qquad (\Delta_1 + k_n^2 - U_{nn})F_n(\vec{r}_1) = U_{no}F_o(\vec{r}_1) \equiv H(\vec{r}_1)$$

where $H(\vec{r}_1)$ is a known function. If the solution of the homogeneous equation

$$(23c) \qquad (\Delta_1 + k_n^2 - U_{nn})F_n(\vec{r}_1) = 0$$

is $\mathcal{F}(r_1, \pi - \Theta)$, then the solution of (23b) for large $\vec{r}_1$ is

$$(24) \qquad F_n(\vec{r}_1) \underset{r_1 \to \infty}{\sim} -\frac{1}{4\pi}\frac{e^{ik_n r_1}}{r_1}\int d\vec{r}_1{}' \, \mathcal{F}_n(\vec{r}_1{}', \pi - \Theta')H(\vec{r}_1{}').$$

The scattered amplitude will then be

$$(25) \qquad f_n(\theta,\phi) = -\frac{1}{4\pi}\int d\vec{r}_1{}' \, \mathcal{F}_n(r_1', \pi - \Theta') \, U_{no}(\vec{r}_1{}')F_o(\vec{r}_1{}')$$

where $F_o(\vec{r}_1{}')$ is the regular solution of (23a) and $U_{no}(\vec{r})$ is given by (10).

Massey[6] points out that in order to include exchange in this approximation, one can use the close coupling treatment. In this case, instead of using (6) as an expansion for the wave function $\Psi(\vec{r}_1,\vec{r}_2)$, we use a different form. Since we are considering two electrons, $\Psi(\vec{r}_1,\vec{r}_2)$ is either symmetrical or antisymmetrical depending on whether the spins of the electrons are parallel or antiparallel. We assume, then, that to a good approximation, $\Psi(\vec{r}_1,\vec{r}_2)$ is:

$$\Psi(\vec{r}_1,\vec{r}_2) = F_o^{\pm}(\vec{r}_1)\Phi_o(\vec{r}_2) \pm F_o^{\pm}(\vec{r}_2)\Phi_o(\vec{r}_1) + F_n^{\pm}(\vec{r}_1)\Phi_n(\vec{r}_2) \pm F_n^{\pm}(\vec{r}_2)\Phi_n(\vec{r}_1). \tag{26}$$

The calculation has been applied to the excitation from the 1S to the 2S-state of hydrogen. Massey[7] shows that in this case, one is led to the following expression for the scattered amplitude

$$\begin{aligned} f_1^{\pm}(\theta,\Phi) &= -\frac{1}{4\pi}\int \mathcal{F}_1^{\pm}(r_1,\pi-\Theta_1)U_{10}(r_1)\mathcal{F}_o^{\pm}(\vec{r}_1)d\vec{r}_1 \\ &\mp \frac{1}{4\pi}\int d\vec{r}_1 d\vec{r}_2\, \mathcal{F}_1^{\pm}(r_1,\pi-\Theta_1)K_{10}(r_1,r_2)\mathcal{F}_o(\vec{r}_2) \end{aligned} \tag{27}$$

where

$$U_{10}(r_1) = 2\int \Phi_o^{*}(r_2)\Phi_1(r_2)\left\{\frac{2}{r_{12}} - \frac{2}{r_1}\right\} d\vec{r}_2 \tag{28a}$$

$$K_{10}(r_1,r_2) = \Phi_1(r_1)\Phi_o(r_2)\left\{k_1^2 - \frac{2}{r_{12}} - 2E_o\right\} \tag{28b}$$

and $\mathcal{F}_o^{\pm}$ and $\mathcal{F}_1^{\pm}$ are distorted waves. In order to proceed further, Massey[7] carries out a spherical harmonic analysis of $\mathcal{F}_o$ and $\mathcal{F}_1$ and points out that only the zero order cross section has been calculated. In this case, the equation satisfied by $\mathcal{F}_{o,o}^{\pm}$ is

$$(29) \qquad \left\{\frac{d^2}{dr^2} + k_o^2 - U_{oo}\right\}(r\mathcal{F}^{\pm}_{oo}) \pm \int K^{o}_{oo}(r,r')r'\mathcal{F}^{\pm}_{o,o}(r')dr' = 0$$

with a similar equation for $\mathcal{F}^{\pm}_{1,0}$. Here

$$K^{o}_{oo}(r,r') = 4\pi rr'\Phi_o(r)\Phi_o(r')\left\{-2\gamma_o(r,r') + k_o^2 - 2E_o\right\}$$

where

$$\begin{aligned} \gamma_o(r,r') &= \frac{1}{r'} \qquad && r' > r \\ &= \frac{1}{r} . && r' < r . \end{aligned}$$

The functions $\mathcal{F}^{\pm}_{o,o}$ and $\mathcal{F}^{\pm}_{1,0}$ cannot be obtained directly and must be obtained by assuming a trial function which asymptotically behaves as

$$\mathcal{F}^{\pm}_{o,o} \sim A^{\pm}_{o} \frac{1}{r} \sin(k_o r + \eta^{\pm}_{o})$$

$$\mathcal{F}^{\pm}_{0,1} \sim B^{\pm}_{o} \frac{1}{r} \sin(k_1 r + \zeta^{\pm}_{o})$$

where η_o and ζ_o are the zeroth order phase shifts. The results of these calculations show that a maximum occurs at about 13.5 e.v. However, the magnitude of the calculated cross section as given by Massey, $0.714\pi a_o^2$, is about ten times larger than the experimental value, $6 \times 10^{-2}\pi a_o^2$.

3. Impulse approximation: fundamental theory

We now derive the various formulas we need for our calculations. The Schrödinger equation for the problem

$$(1) \qquad H\,\Psi(\vec{r}_1,\vec{r}_2) = E\,\Psi(\vec{r}_1,\vec{r}_2)$$

where $\vec{r}_1$ and $\vec{r}_2$ are the position vector of the incident and bound electrons respectively and E is the total energy of the system given by:

(2) $$E = \frac{\hbar^2 k_1^2}{2m} - |\epsilon|$$

where $\vec{k}_1$ is the wave number of the incident electron and ϵ the binding energy of the ground state of hydrogen. H is the Hamiltonian of the system

(3) $$H = -\frac{\hbar^2}{2m}\Delta_1 - \frac{\hbar^2}{2m}\Delta_2 - \frac{e^2}{r_1} - \frac{e^2}{r_2} + \frac{e^2}{r_{12}} .$$

We desire a solution of the form

(4) $$\Psi(\vec{r}_1,\vec{r}_2) = \Psi_i(\vec{r}_1,\vec{r}_2) + \Psi_s(\vec{r}_1,\vec{r}_2).$$

Here $\Psi_i(\vec{r}_1,\vec{r}_2)$ represents the initial state of the system and is given by

(5) $$\Psi_i(\vec{r}_1,\vec{r}_2) = (2\pi)^{-3/2}\, e^{i\vec{k}_1\cdot\vec{r}_1}\, \Phi_o(\vec{r}_2)$$

where $e^{i\vec{k}_1\cdot\vec{r}_1}$ represents electron (1) as an incident plane wave of momentum $\vec{k}_1$ and $\Phi_o(\vec{r}_2)$ is the wave function describing the ground state of hydrogen. $\Psi_s(\vec{r}_1,\vec{r}_2)$ represents the final state of the system and contains various kinds of outgoing waves and is given by

(6) $$\Psi_s(\vec{r}_1,\vec{r}_2) = \int G(\vec{r}_1,\vec{r}_2;\vec{r}_1{}',\vec{r}_2{}')\, V\, \Psi(\vec{r}_1{}',\vec{r}_2{}')\, d\vec{r}_1{}'\, d\vec{r}_2{}'$$

where $G(\vec{r}_1,\vec{r}_2;\vec{r}_1{}',\vec{r}_2{}')$ is the Green's function for the equation

(7) $$(H_o - E)\, \Psi(\vec{r}_1,\vec{r}_2) = 0$$

with

(8) $$H_o = -\frac{\hbar^2}{2m}\Delta_1 - \frac{\hbar^2}{2m}\Delta_2 - \frac{e^2}{r_2} .$$

A Green's function[8] for our problem is

(9) $$G(\vec{r}_1,\vec{r}_2;\vec{r}_1{}',\vec{r}_2{}') = -\frac{m}{2\pi\hbar^2}\sum_n \Phi_n(\vec{r}_2)\Phi_n(\vec{r}_2{}')\, \frac{e^{ik_n'|\vec{r}_1-\vec{r}_1{}'|}}{|\vec{r}_1 - \vec{r}_1{}'|}$$

where the sum includes an integral over the continuum states and

(10) $$k_n'^2 = \frac{2m}{\hbar^2}(E-E_n).$$

For large r_1, we then have, upon substitution of (9) into (6),

(11) $$\Psi_s(\vec{r}_1,\vec{r}_2) \underset{r_1 \to \infty}{\sim} -\frac{m}{2\pi\hbar^2}\sum_n \Phi_n(\vec{r}_2)\frac{e^{ik_n' r_1}}{r_1} \int d\vec{r}_1{}' \, d\vec{r}_2{}' \, \Phi_n^*(\vec{r}_2{}') e^{-i\vec{k}_n'\cdot\vec{r}_1{}'} V \, \Psi(\vec{r}_1{}',\vec{r}_2{}').$$

For exchange, we take the limit as r_2 approaches ∞, and this leads to:

(12) $$\Psi_s(\vec{r}_1,\vec{r}_2) \underset{r_2 \to \infty}{\sim} -\frac{m}{2\pi\hbar^2}\sum_n \Phi_n(\vec{r}_1)\frac{e^{ik_n' r_2}}{r_2} \int d\vec{r}_1{}' \, d\vec{r}_2{}' \, \Phi_n^*(\vec{r}_1{}') e^{-i\vec{k}_n'\cdot\vec{r}_2{}'} V \, \Psi(\vec{r}_1{}',\vec{r}_2{}').$$

In these equations, Φ_n represents the wave function of the electron in the field of the proton in the state n. We assume the following approximate form for $\Psi(\vec{r}_1,\vec{r}_2)$

(13) $$\Psi(\vec{r}_1,\vec{r}_2) \longrightarrow \Psi_a(\vec{r}_1,\vec{r}_2) = \int d\vec{k}_2 \, g_o(\vec{k}_2) \, \Psi_{\vec{k}_1,\vec{k}_2}(\vec{r}_1,\vec{r}_2).$$

Here $g_o(\vec{k}_2)$ is the Fourier transform of the hydrogen atom ground state wave function. $\Psi_{\vec{k}_1,\vec{k}_2}(\vec{r}_1,\vec{r}_2)$ is a wave function representing the interaction of an electron of momentum $\vec{k}_1$ by a free electron of momentum $\vec{k}_2$. What we have done in (13) is to replace the bound electron by a free electron whose momentum distribution is equivalent to the ground state wave function and consider its interaction with the incident electron.

The substitution of (13) into (12), gives

$$\Psi_s^{(d)}(\vec{r}_1,\vec{r}_2) \underset{r_1 \to \infty}{\approx} -\frac{2m}{4\pi\hbar^2}\sum_n \int d\vec{k}_2 \Phi_n(\vec{r}_2)\, \frac{e^{ik_n r_1}}{r_1}\, g_o(\vec{k}_2)$$

(14)

$$\iint d\vec{r}_1{}' d\vec{r}_2{}'\, e^{-i\vec{k}_n{}'\cdot\vec{r}_1{}'}\, \Phi_n^*(\vec{r}_2{}') V\, \Psi_{\vec{k}_1\vec{k}_2}(\vec{r}_1{}',\vec{r}_2{}').$$

For exchange, we take the limit as r_2 approaches ∞

$$\Psi_s^{(e)}(\vec{r}_1,\vec{r}_2) \underset{r_2 \to \infty}{\approx} -\frac{2m}{4\pi\hbar^2}\sum_n \int d\vec{k}_2 \Phi_n(\vec{r}_1)\, \frac{e^{ik_n r_2}}{r_2}\, g_o(\vec{k}_2)$$

(15)

$$\iint d\vec{r}_1{}' d\vec{r}_2{}'\, e^{-i\vec{k}_n{}'\cdot\vec{r}_2{}'}\, \Phi_n^*(\vec{r}_1{}') V\, \Psi_{\vec{k}_1\vec{k}_2}(\vec{r}_1{}',\vec{r}_2{}') .$$

We can represent the scattered amplitude by an R-matrix. In our case, this is

(16) $$(\vec{k}_1{}',n\,|R_{12}|\vec{k}_1,\vec{k}_2) = -i \iint d\vec{r}_1 d\vec{r}_2\, e^{-i\vec{k}_n{}'\cdot\vec{r}_1}\Phi_n(\vec{r}_2) V\, \Psi_{\vec{k}_1\vec{k}_2}(\vec{r}_1,\vec{r}_2).$$

The R-matrix represents the matrix elements of the perturbing potential between the initial and final states of the process and is related to the scattering cross section.

In order to derive the relation between the R-matrix and the scattering cross section, we use the time-dependent scattering theory developed by Gell-Mann and Goldberger[9]. Our system is described by the following equation ($\hbar = 1$)

(17) $$i\frac{\partial}{\partial t}\Psi(t) = H\,\Psi(t)$$

where H is the Hamiltonian and $\Psi(t)$ the wave function of the system composed of an electron and a hydrogen atom. We separate H into two terms by

(18) $$H = H_1 + H_2$$

where H_1 is the Hamiltonian describing the system when the interaction between the incident electron and the hydrogen atom is cut-off and H_2 represents the interaction terms. Thus,

$$H_1 = -\frac{1}{2m}\Delta_1 - \frac{1}{2m}\Delta_2 - \frac{e^2}{r_2} \tag{18a}$$

$$H_2 = -\frac{e^2}{r_1} + \frac{e^2}{r_{12}} \quad . \tag{18b}$$

The non-interacting state can then be represented by the equation

$$i\,\frac{\partial\Phi(t)}{\partial t} = H_1\Phi(t) \ . \tag{18c}$$

The purpose of $\Phi(t)$ is to characterize $\Psi(t)$.

We are interested in transitions from the inital state Φ_i to the final state Φ_j. If the system was in the state Φ_i at an infinite time in the past, we can assume that Ψ_i can be described by

$$\Psi_i(t) = e^{+iH(T-t)}\Phi_i(T) \ . \tag{19}$$

Equation (19) implies that the incident wave is released suddenly into the system. Actually, the beam is prepared in some way and is fed into the system over a period of time. To account for this fact, instead of using (19), we use a statistical average of waves of the form (19) over a period of time T_o and take the limit as $T_o \to \infty$. This leads to

$$\Psi_i(t) = \lim_{T_o \to \infty} \frac{1}{T_o} \int_{-T_o}^{0} dT e^{iH(T-t)}\Phi_i(T) \quad . \tag{20}$$

Writing $\epsilon = 1/T_o$,

$$\Psi_i^{(\epsilon)}(t) = \epsilon \int_{-\infty}^{0} dT\, e^{\epsilon T}\, e^{iH(T-t)}\, \Phi_i(T) \quad , \tag{21}$$

remembering that, in all evaluation of the cross sections, we take the limit as $\epsilon \to 0$. The Φ's are normalized in a cube of side L and volume L^3. Since $T_o = L/v$ where v is the group velocity, it follows that the limit $\epsilon \to 0$ and $L \to \infty$ must be taken simultaneously. Furthermore, as $\epsilon \to 0$ and $L \to \infty$, $\epsilon^{-1}L^{-3} \to 0$.

We must now derive the rate at which transitions are taking place from the state i to the state j. The probability for transition from a state i to a state j is:

$$W_{ij}(t) = \frac{|f_{ij}|^2}{N_j} \tag{22}$$

where

$$f_{ij}(t) = < \Phi_j(t) | \Psi_i(t) > \tag{22a}$$

$$N_j = < \Psi_j(t) | \Psi_i(t) > \quad . \tag{22b}$$

Let

$$\Phi_i(t) = e^{-iE_i t} \Phi_i$$

then (18c) gives

$$(H_1 - E_i) \Phi_i = 0 \; . \tag{23}$$

Equation (21) then becomes:

$$\Psi_i^\epsilon(t) = \epsilon \int_{-\infty}^{\epsilon} dT \, e^{-iHt} e^{\epsilon T} e^{i(H-E_i)T} \Phi_i = e^{-iHt} \frac{\epsilon}{\epsilon + i(H-E_i)} \Phi_i \; . \tag{24}$$

But Φ_i is an eigenfunction of H_1 and, if we consider H operating on Φ_i, we have

$$H\Phi_i = (H_1 + H_2) \Phi_i$$

$$= (E_i + H_2) \Phi_i$$

or

$$(H - E_i) \Phi_i = H_2 \Phi_i \; . \tag{25}$$

Then at t = 0,

$$\Psi_i^{(\epsilon)}(0) = \frac{\epsilon}{\epsilon+i(H-E_i)}\,\Phi_i = \left[1 + \frac{H - E_i}{E_i-H+i\epsilon}\right]\Phi_i$$

or

$$\Psi_i^{(\epsilon)}(0) = \Phi_i + \frac{1}{E_i-H+i\epsilon}\,H_2\Phi_i \tag{26}$$

using (25). Instead of (26), we have, by solving for Φ_i

$$\Phi_i = \Psi_i^{(\epsilon)} - \frac{H_2}{E_i-H_1+i\epsilon}\,\Psi_i^{(\epsilon)}$$

or

$$\Psi_i^{(\epsilon)}(0) = \Phi_i + \frac{1}{E_i-H_1+i\epsilon}\,\Psi_i^{(\epsilon)}(0) \;. \tag{27}$$

Thus

$$\begin{aligned} f_{ij}(0) &= < \Phi_j|\Psi_i^{(\epsilon)}(0) > \\ &= \delta_{ij} + < \Phi_j|\, \frac{1}{E_i-H_1+i\epsilon}|\Psi_i^{(\epsilon)}(0) > \qquad (28)\\ &= \delta_{ij} + \frac{1}{E_i-E_j+i\epsilon}\,R_{ij}(\epsilon) \end{aligned}$$

where

$$R_{ij}(\epsilon) = < \Phi_j|H_2|\Psi_i^{\epsilon}(0) > \;. \tag{29}$$

If we expand (27) in a power series of Φ_i, we see that the term $\frac{1}{E_i-H_1+i\epsilon}$ acts only on $V\Phi_i$ and not on Φ_i directly. Thus, R_{ij} is a well-behaved function of the energy. Further, since R_{ij} is proportional to L^{-3}, due to the normalization of the Φ's, it follows that as $\epsilon \to 0$ and $L \to \infty$,

$$R_{ij}(\epsilon)L^3 \to R_{ij}. \tag{30}$$

We mentioned above that we were interested in the rate of transitions, that is, $\frac{dW_{ij}}{dt}$. To calculate this, we need the time derivatives of f_{ij}. We write

$$f_{ij}(t) = < \Phi_j|e^{i(E_i-H)t}|\Psi_i^{(\epsilon)}(0) > , \tag{31a}$$

Then

$$\frac{df_{ij}(0)}{dt} = i < \Phi_j | E_j - H | \Psi^{(\epsilon)}(0) >$$

(31b) $$= - i < \Phi_j | H_2 | \Psi_i^{(\epsilon)}(0) >$$

$$= - i R_{ij}(\epsilon) .$$

Since from equation (22),

$$\frac{dW_{ij}}{dt}\Big]_{t=o} = \frac{1}{N_i} \frac{d}{dt} |f_{ij}(t)|^2\Big]_{t=o}$$

we must calculate $\frac{d}{dt} |f_{ij}(t)|^2$. We have

$$\frac{d}{dt}|f_{ij}(t)|^2\Big]_{t=o} = \dot{f}_{ij}(0) f^*_{ij}(0) + f_{ij}(0) \dot{f}^*_{ij}(0)$$

where the dot denotes differentiation with respect to time.

Using (28) and (31), we obtain

(32) $$\frac{d}{dt} |f_{ij}(t)|^2\Big]_{t=o} = 2\delta_{ij} \mathrm{Im} R_{ij}(\epsilon) + \frac{2}{(E_j - E_i)^2 + \epsilon^2} |R_{ij}(\epsilon)|^2 .$$

We must now deal with N_i. The Φ's form a complete set of states. Hence, if we compute $\sum_j |f_{ij}(t)|^2$ from equation (31a), we obtain

(33) $$\sum_j |f_{ij}(t)|^2 = N_i .$$

Furthermore, N_i is a normalization constant and hence independent of time. It follows that if we take the time derivative of (33) at t = 0, we have

(34) $$2 \mathrm{Im} R_{jj}(\epsilon) + \sum_j \frac{2\epsilon}{(E_i - E_j)^2 + \epsilon^2} |R_{ij}(\epsilon)|^2 = 0 .$$

Thus

$$N_j = 1 + \frac{1}{} I_m R_{jj}(\epsilon)$$

by using (28) and (34). Now as $\epsilon \to 0$ and $L \to \infty$ we see that $N_j \to 1$.

Thus, the transition rate is

(35) $$W_{ij}(0) = 2\delta_{ij} I_m R_{ij}(\epsilon) + \frac{2\epsilon}{(E_j - E_i)^2 + \epsilon^2} |R_{ij}(\epsilon)|^2 .$$

The scattering cross section is equal to the transition rate divided by the initial flux. In our case the initial flux is vL^{-3} where v is the velocity of the incoming electron. Hence,

$$\sigma_{ij} = \lim_{\substack{\epsilon \to 0 \\ L \to \infty}} \frac{2\epsilon}{(E_j - E_i)^2 + \epsilon^2} |R_{ij}(\epsilon)|^2 \frac{L^3}{v} .$$

As $\epsilon \to 0$, the factor $2\epsilon/(E_j-E_i)^2+\epsilon^2 \to 2\pi\delta(E_j-E_i)$, and by using (30) we obtain

$$(36) \qquad \sigma_{ij} = \frac{2\pi}{v} |R_{ij}|^2 \delta(E_j - E_i) .$$

This is the relation between the R-matrix and the cross section that we sought.

Let us go back to equation (16). The potential V consists of two terms

$$- \frac{e^2}{r_1} + \frac{e^2}{r_{12}} .$$

Substituting into (16),we obtain

$$(\vec{k}'_n, n|R_{12}|\vec{k}_1,\vec{k}_2) = - ie^2 \iint d\vec{r}_1 d\vec{r}_2 e^{-i\vec{k}'_n \cdot \vec{r}_1} \Phi_n(\vec{r}_2)(- \frac{1}{r_1} + \frac{1}{r_{12}}) \Psi_{\vec{k}_1\vec{k}_2}(\vec{r}_1\vec{r}_2) .$$

If we were to use the exact wave functions for the bound electron in the final state, i.e., Coulombic wave functions, the integration over $\vec{r}_2$ would yield zero when we compute the matrix element involving $1/r_1$ since the wave functions in the initial and final states are orthogonal. Thus, it would seem that the wave originating at the proton does not contribute to the inelastic scattering; the only effect of the proton, which we assume to have infinite mass, is to deflect the incident electron into a new direction. Thus, in inelastic processes, the wave originating at the proton does not contribute to the scattering cross sections.

One further simplification will be made. Instead of using hypergeometric functions to describe the electrons in the continuum , we will use plane waves for ionization. The integrals are intractable, otherwise.

One immediate effect of this last simplification can be seen very quickly. Looking back at (16) and putting $\Phi_n(r_2) = e^{i\vec{k}_2 \cdot \vec{r}_2}$ we see that the

R-matrix in the case of direct scattering is

$$(\vec{k}_1',\vec{k}_2'|R_{12}^{(d)}|\vec{k}_1,\vec{k}_2) = -i\iint d\vec{r}_1 d\vec{r}_2 e^{-i\vec{k}_1'\cdot\vec{r}_1 - i\vec{k}_2'\cdot\vec{r}_2} V\Psi_{\vec{k}_1\vec{k}_2}(\vec{r}_1,\vec{r}_2) ,$$

while, for exchange,

$$(\vec{k}_1',\vec{k}_2'|R_{12}^{(e)}|\vec{k}_1,\vec{k}_2) = -i\iint d\vec{r}_1 d\vec{r}_2 e^{-i\vec{k}_1'\cdot\vec{r}_2 - i\vec{k}_2'\cdot\vec{r}_1} V\Psi_{\vec{k}_1\vec{k}_2}(\vec{r}_1,\vec{r}_2) .$$

These two expressions are exactly the same except that we have interchanged $\vec{r}_1$ and $\vec{r}_2$ or, by the same token, $\vec{k}_1$ and $\vec{k}_2$. This will then have no effect on the final value of the integrals. The two electrons are being treated identically and we cannot distinguish between singlet and triplet scattering. The main difference between the correct wave function and a plane wave is the fact that in the latter, the singularity at the origin, in the wave function, is absent. The effect of this approximation has not been estimated. Since our results compared favorably with the experimental data available, we rely upon these for our justification in using this approximation.

We factor $\Psi_{\vec{k}_1\vec{k}_2}(\vec{r}_1\vec{r}_2)$ into the product of two functions, one representing the motion of the center of mass and the other, the relative motion with respect to the center of mass:

$$\Psi_{\vec{k}_1\vec{k}_2}(\vec{r}_1,\vec{r}_2) = (2\pi)^{-3/2} e^{\frac{i}{2}(\vec{k}_1+\vec{k}_2)\cdot(\vec{r}_1+\vec{r}_2)} H_{\frac{1}{2}(\vec{k}_1-\vec{k}_2)}(\vec{r}_1-\vec{r}_2) .$$

Thus, (16) becomes

$$(\vec{k}'_1 n|R_{12}|\vec{k}_1,\vec{k}_2) = \frac{-ie^2}{(2\pi)^{3/2}}\iint d\vec{r}_1 d\vec{r}_2 e^{-i\vec{k}_1'\cdot\vec{r}_1}\Phi_n^*(\vec{r}_2)\frac{1}{r_{12}} e^{+\frac{i}{2}(\vec{k}_1+\vec{k}_2)(\vec{r}_1+\vec{r}_2)}$$

$$H_{\frac{1}{2}(\vec{k}_1-\vec{k}_2)}(\vec{r}_1-\vec{r}_2) .$$

Substituting for $\Phi_n(\vec{r}_2)$ its Fourier transform, we get

$$(37)\qquad (\vec{k}_1', n|R_{12}|\vec{k}_1,\vec{k}_2) = e^2\int d\vec{k}_2''\, g_n^*(\vec{k}_2'')(\vec{k}_1',\vec{k}_2''\,|R_{12}|\vec{k}_1,\vec{k}_2)$$

where

$$(38)\qquad (\vec{k}_1',\vec{k}_2''|R_{12}|\vec{k}_1,\vec{k}_2) = -\frac{i}{(2\pi)^3}\iint \frac{d\vec{r}_1 d\vec{r}_2}{r_{12}} \exp\left\{-i\vec{k}_1'\cdot\vec{r}_1 - i\vec{k}_2''\cdot\vec{r}_2 + \tfrac{1}{2}i(\vec{k}_1+\vec{k}_2)\cdot(\vec{r}_1+\vec{r}_2)\right\} H_{\frac{1}{2}(\vec{k}_1-\vec{k}_2)}(\vec{r}_1-\vec{r}_2).$$

We now carry out the transformation

$$\vec{r}_1 - \vec{r}_2 = \vec{r} \qquad\qquad \tfrac{1}{2}(\vec{r}_1 + \vec{r}_2) = \vec{\rho}\ .$$

This leads to

$$(\vec{k}_1',\vec{k}_2''\,|R_{12}|\vec{k}_1,\vec{k}_2) = -\frac{i}{(2\pi)^3}\int d\vec{\rho}\,\exp\left\{-i(\vec{k}_1'+\vec{k}_2''-\vec{k}_1-\vec{k}_2)\cdot\vec{\rho}\right\}\int\frac{d\vec{r}}{r}\,e^{-i\vec{k}_1'\cdot\vec{r}_1}H_k(\vec{r})$$

$$(39)\qquad = \delta(\vec{k}_1' + \vec{k}_2'' - \vec{k}_1 - \vec{k}_2)(\vec{k}'|r|\vec{k})$$

where

$$\vec{k} = \frac{1}{2}(\vec{k}_1-\vec{k}_2)$$
$$\vec{k}' = \frac{1}{2}(\vec{k}_1'-\vec{k}_2'')$$

and

$$(40)\qquad (\vec{k}'|r|\vec{k}) = -i\int\frac{d\vec{r}}{r}\,e^{-i\vec{k}'\cdot\vec{r}}\,H_{\vec{k}}(\vec{r})\ .$$

The R-matrix describing the inelastic collision will then be

$$(41)\qquad (\vec{k}_1',n|R|\vec{k}_1,0) = \iint d\vec{k}_2''\,d\vec{k}_2'''g_n^*(\vec{k}_2'')(\vec{k}_1',\vec{k}_2''\,|\,R_{12}|\vec{k}_1,\vec{k}_2''')g_0(\vec{k}_2''')\ .$$

Substituting (39) into (41) and carrying out the $\vec{k}_2''$ integration leads to

$$(42)\qquad (\vec{k}_1'n|R|\vec{k}_1,0) = e^2\int d\vec{k}_2''\,g_n^*(\vec{k}_2'')(\vec{k}'|r|\vec{k})g_0(\vec{k}_1'+\vec{k}_2''-\vec{k}_1).$$

For ionization, the R-matrix is obtained by letting n correspond to $\vec{k}_2'$. $g_n(\vec{k}_2'')$ will then be the Fourier transform of a plane wave. Thus

(43) $$(\vec{k}_1', \vec{k}_2' | R_{ion} | \vec{k}_1, 0) = e^2 \int d\vec{k}_2'' \, g^*_{\vec{k}_2'}(\vec{k}_2'')(\vec{k}'|r|\vec{k}) g_o(\vec{k}_1' + \vec{k}_2'' - \vec{k}_1).$$

For excitation to the 2P and 2S states, equation (42) is applied directly. For exchange, we see from (12) that in the case of ionization, the only effect is to interchange $\vec{r}_1$ and $\vec{r}_2$ in the final state. Since we are using plane waves, there is no distinction between the two scattering processes. For the 2S and 2P states, we have

(44) $$(\vec{k}_1' \, , \, n|R_{ex}|k_1, 0) = - ie^2 \int d\vec{k}_2 g_o(\vec{k}_2) g_n^*(\vec{k}_1' + \vec{k}_2 - \vec{k}_1) \int \frac{d\vec{r}}{r} e^{i\vec{k}\cdot\vec{r}} H_k(\vec{r}).$$

Before we proceed to compute the cross sections we consider the r-matrix. This is given by (40). $H_{\vec{k}}(\vec{r})$ represents the interaction of two free electrons and is given by [10]

(45) $$H_k(\vec{r}) = N(k) e^{i\vec{k}\cdot\vec{r}} F(- i/2a_o k; 1; ikr - i\vec{k}\cdot\vec{r})$$

where F is the hypergeometric of its argument and

(46) $$N(k) = \sqrt{\frac{m}{\hbar k}} \, \Gamma(1 + i/2a_o k) e^{- \pi/4a_o k} ,$$

where $\Gamma(1+i/2a_o k)$ is the gamma function

Thus (40) becomes

(47) $$(\vec{k}'|r|\vec{k}) = - iN(k)I$$

with

(48) $$I = \int \frac{d\vec{r}}{r} e^{i(\vec{k}-\vec{k}')\cdot\vec{r}} F(- i/2a_o k; 1; ikr - i\vec{k}\cdot\vec{r}) .$$

We rewrite this integral as

(49) $$I = \int \frac{d\vec{r}}{r} e^{i\vec{q}\cdot\vec{r}} F(- in; 1; ikr - i\vec{k}\cdot\vec{r}).$$

Nordsieck [11] has evaluated this integral for the case in which an exponential factor of the form $e^{-\lambda r}$ occurs in the integrand. We have evaluated this integral in Appendix A and the result is

(50) $$I = \frac{4\pi}{q^2} \left(\frac{q^2 - 2\vec{q}\cdot\vec{k}}{q^2}\right)^{in} .$$

We will now proceed to apply the above formulas to the cases we have under consideration.

4. Ionization cross section

The R-matrix for ionization is given in equation (3.43) which states that

(1) $$(\vec{k}_1', \vec{k}_2'|R_{ion}|\vec{k}_1 0) = e^2 \int d\vec{k}_2'' \, (\vec{k}'|r|\vec{k}) g^*_{\vec{k}_2'}(\vec{k}_2'') g_o(\vec{k}_1' + \vec{k}_2'' - \vec{k}_1)$$

with $(\vec{k}'|r|\vec{k})$ given by (3.47) combined with (3.50). Substituting the values of $\vec{q}$ and n into these equations, we obtain

(2) $$(\vec{k}'|r|\vec{k}) = \frac{4\pi i}{|\vec{k}-\vec{k}'|^2} N(k) \left\{ \frac{2\vec{k}\cdot(\vec{k}-\vec{k}') - (\vec{k}-\vec{k}')^2}{|\vec{k}-\vec{k}'|^2} \right\}^{i/2a_o k} .$$

Let us now compute $g_{\vec{k}_2'}(\vec{k}_2'')$ and $g_o(\vec{k}_2'+\vec{k}_2'' \vec{k}_1)$. We recall that

(3) $$g_m(\vec{\lambda}) = \frac{1}{(2\pi)^{3/2}} \int d\vec{r} \, e^{-i\vec{\lambda}\cdot\vec{r}} \, \Phi_m(\vec{r})$$

where $\Phi_m(\vec{r})$ is the wave function of the bound electron and the subscript m indicates the state. For the final state, we are using a plane wave. Hence

(4) $$\begin{aligned} g_{\vec{k}_2}(\vec{k}_2'') &= \frac{1}{(2\pi)^3} \int d\vec{r} \, e^{-i\vec{k}_2''\cdot\vec{r} + i\vec{k}_2\cdot\vec{r}} \\ &= \delta(\vec{k}_2' - \vec{k}_2''). \end{aligned}$$

The ground-state wave function $\Phi_o(\vec{r})$ is

$$\Phi_o(\vec{r}) = \frac{1}{(4\pi a_o^3)^{1/2}} e^{-r/a_o} .$$

Hence

(5) $$g_o(\vec{k}_1' + \vec{k}_2'' - \vec{k}_1) = \frac{\sqrt{2}}{\pi\left\{1+a_o^2|\vec{k}_1'+\vec{k}_2'' - \vec{k}_1|^2\right\}^2} .$$

Substituting (4) and (5) into (1), the $\vec{k}_2''$-integration can be carried through, yielding

$$(6)\quad (\vec{k}_1',\vec{k}_2'|R_{ion}|\vec{k}_1,0) = \frac{e^2\sqrt{2}}{\pi}\,\frac{(\vec{k}'|r|\vec{k})}{\left\{1+a_o^2|\vec{k}_1'+\vec{k}_2'-\vec{k}_1|^2\right\}^2}\,.$$

Combining (2) and (6) and substituting into (3.36) we obtain for the differential scattering cross section

$$(7)\quad \sigma_{ion}d\vec{k}_1 d\vec{k}_2' = \frac{2^8\pi^3 m^3 e^4}{\hbar^4 a_o k_1}\,\frac{\exp\left[-\pi/a_o|2\vec{k}_1-\vec{k}_1'-\vec{k}_2'|\right]}{\sinh\left[\pi/a_o|2\vec{k}_1-\vec{k}_1'-\vec{k}_2'|\right]} \times\frac{\delta(E_1'+E_2'-E)d\vec{k}_1'd\vec{k}_2'}{|\vec{k}_1-\vec{k}_1'|^4|2\vec{k}_1-\vec{k}_1'-\vec{k}_2'|^2\left[1+a_o^2|\vec{k}_1-\vec{k}_1'-\vec{k}_2'|^2\right]^4}\,.$$

The total cross section will be

$$\sigma_t = \int\int \sigma_{ion}\, d\vec{k}_1'd\vec{k}_2'.$$

Before we proceed to the evaluation of this double integral, a word must be said about the limits of integration. Due to the δ-function appearing in the integrand of (7), the values of E_2' and hence k_2' are restricted by the relation

$$k_2'^2 = k_1^2 - \vec{1} - k_1'^2\quad .$$

Hence the range of k_2' will have to extend over the entire space of k_2'. We must be careful in dealing with the δ-function. It involves the square of the magnitude of k_2' rather than k_2'. This is dealt with by using the relation

$$\delta(x^2-a^2) = \frac{1}{2a}\left(\delta(x-a)+\delta(x+a)\right).$$

(This point is dealt with in Appendix B.) The remaining problem is the magnitudes of k_1'. Again the angular integrations can be dealt with by substitution of variables. This is done in Appendix B. The range of k_1' is fixed by conservation of energy. Two extreme cases occur - one in which the hydrogen atom is barely ionized. The incident electron then carries off the entire energy and $k_1'^2 = k_1^2 - 1$. At the other end, the emerging electron carries off the entire energy and thus $k_1'^2 = 0$.

The integration is carried out in Appendix B and leads to

$$\sigma_t = \frac{2^9\pi^3}{k_1^2}\left\{ -\frac{64}{15}\,\sigma_1 + \frac{8}{5}\,\sigma_2 + \frac{4}{15}\,\sigma_3 + \frac{7}{3}\,\sigma_4 + 7\sigma_5 - 7\sigma_6 \right\}$$

where the σ's are defined in the appendix. The integrals σ' cannot be carried out analytically. They were integrated numerically. The results are plotted in Figure 1. The curves are drawn in this figure and are labeled according to the calculation they are based upon. The Born approximation was computed numerically by Fite who used the Mott and Massey formula given in Section 2. The maximum occurs at 20 volts instead of 98 volts and gives a fairly large value, namely $1.2\pi a_o^2$. This is much larger than the experimental value. Our curve, on the other hand, gives a maximum of $0.55\pi a_o^2$ at an energy of 86 volts and is in fair agreement with the experimental result.

We examine now the behavior of the cross section for high energies. As $k_1 \rightarrow \infty$, the factor $1 + (k_1 - K)^2$ behaves as k_1^2; the factor $e^{-\pi/K}(\sinh \frac{\pi}{K}) \longrightarrow 1$ and thus the cross section behaves a $1/k_1'^{10}$. It is seen that it falls off very rapidly as $k_1 \rightarrow \infty$.

We now examine the behavior at threshold. To this end, we go back to equation (7). We are concerned with the behavior of σ_t as $k_1^2 = 1 + \epsilon$ $(\epsilon \rightarrow 0)$. Since in this limit $\vec{k}_1'$ and $\vec{k}_2'$ are both small, we can write,

$$\sigma_{ion} d\vec{k}_1' d\vec{k}_2' \approx \frac{2^8\pi^3 e^{-\pi/2k_1}}{4k_1^3 \sinh \pi/2k_1} \, \frac{\delta(k_1'^2 + k_2'^2 - \epsilon)}{|\vec{k}_1 - \vec{k}_1'| \left[1 + |\vec{k}_1 - \vec{k}_1' - \vec{k}_2'|^2\right]^4} \, d\vec{k}_1' d\vec{k}_2'$$

We carry out the $\vec{k}_2'$ integration; this leads to

$$\int \sigma_{ion} d\vec{k}_1' d\vec{k}_2' \approx \frac{2^6\pi^3}{k_1^3} \int \frac{d\vec{k}_1'}{|\vec{k}_1 - \vec{k}_1'|^4} (\epsilon - k_1'^2)^{1/2} + O(\epsilon^2).$$

The integral over k_1' can now be carried through. The limits on k_1' are 0 and $\epsilon^{1/2}$. Integrating leads to

$$\sigma_t = \text{const } \epsilon.$$

Wannier[12] derives the threshold law for single ionization and obtains

$$\sigma_t \propto \epsilon^{1.123}$$

Massey points out that on the basis of the available evidence

$$\sigma_t \propto \epsilon \ .$$

Our result is in agreement with Massey's; however, it must be remembered that at threshold our approximation cannot be very accurate.

5. 1S-2S cross section

A. Direct scattered amplitude

In the case of excitation, the R-matrix takes the form

$$(1) \quad (\vec{k}'n|R_d|\vec{k}0) = e^2 \int d\vec{k}_2 \, g_n^*(\vec{k}_2+\vec{k}-\vec{k}')g_o(\vec{k}_2)(\vec{k}_1'|r|\vec{k}_2)$$

where $\vec{k}$ and $\vec{k}'$ are the initial final wave numbers of the incident electron respectively and n and 0 are symbols representing, respectively, the final and initial states of the bound electron and

$$(2a) \qquad \vec{k}_1' = 2\vec{k}' - \vec{k} - \vec{k}_2$$

$$(2b) \qquad \vec{k}_1 = \vec{k} - \vec{k}_2$$

Referring to Appendix A, we have, upon the use of (2),

$$(3) \qquad (\vec{k}_1'|r|\vec{k}_1) = \frac{4\pi N(\vec{k}_1)}{|\vec{k}-\vec{k}'|^2} \left\{ \frac{(\vec{k}-\vec{k}')^2-(\vec{k}-\vec{k}')\cdot(\vec{k}-\vec{k}_2)}{|\vec{k}-\vec{k}_2|^2} \right\}^{1/2} |\vec{k}-\vec{k}_2| \ .$$

In order to carry our work further, we must make one more approximation. It is clear that if we substitute (3) into (1), it would be impossible to carry out the $\vec{k}_2$ integration. Hence, we must attempt to take the r-matrix from under the integral sign. Chew[1] points out that this is a slowly varying matrix. We will therefore substitute for $\vec{k}_2$ in the r-matrix $\vec{k} - \vec{k}'$. This approximation is not necessary in the ionization case. The reason is that the final integral over $\vec{k}_2$ involves a δ-function of $\vec{k}_2$ since the final state of the emitted electron is represented by a plane wave. If we had used exact wave functions, the same approximation would have been made. Thus, equation (1) becomes

$$(4) \qquad (\vec{k}'\, n|R_d|\vec{k}0) = -\frac{4\pi e^2 N(k')}{|\vec{k}-\vec{k}'|^2}\left\{\frac{(\vec{k}-\vec{k}')\cdot(\vec{k}+2\vec{k}')}{(\vec{k}-\vec{k}')^2}\right\}^{i/2a_o k'}\int d\vec{k}_2 g_o(\vec{k}_2) g_n^*(\vec{k}+\vec{k}_2-\vec{k}').$$

We recall that

$$(5a) \qquad g_o(\vec{k}_2) = (2\pi)^{-3/2}\int d\vec{r}\, e^{-i\vec{k}_2\cdot\vec{r}}\, \Phi_o(\vec{r})$$

and

$$(5b) \qquad g_n(\vec{k}+\vec{k}_2-\vec{k}') = (2\pi)^{-3/2}\int d\vec{r}\, e^{-i(\vec{k}+\vec{k}_2-\vec{k}')\cdot\vec{r}}\, \Phi_n(\vec{r}) .$$

Hence

$$(6) \qquad \int d\vec{k}_2 g_o(\vec{k}_2) g_n^*(\vec{k}+\vec{k}_2-\vec{k}') = \int d\vec{r}\int d\vec{r}'\,\Phi_o(\vec{r})\Phi_n^*(\vec{r}')e^{i(\vec{k}+r-\vec{k}'\cdot\vec{r}')}(2\pi)^{-3}\int d\vec{k}_2 e^{i\vec{k}_2\cdot(\vec{r}-\vec{r}')}$$

$$= \int d\vec{r}\,\phi_n^*(\vec{r})e^{i(\vec{k}-\vec{k}')\cdot\vec{r}}\Phi_o(\vec{r}).$$

This integral is evaluated in Appendix C; one then obtains for the direct 1S-2S cross section

$$(7) \qquad (\vec{k}',200|R_d|\vec{k},100) = -\frac{2^{19/2}\pi e^2 a_o^2 N(k')}{\left[a+4a_o^2|\vec{k}-\vec{k}'|^2\right]^3}\cdot\left\{\frac{(\vec{k}-\vec{k}')\cdot(\vec{k}+2\vec{k}')}{(\vec{k}-\vec{k}')^2}\right\}^{i/2a_o k'}$$

B. Exchange scattered amplitude

In this case we evaluate equation (2.42) which is

$$(8) \qquad (\vec{k}'200|R_{ex}|\vec{k},100) = -ie^2\int d\vec{k}_2 g_o(\vec{k}_2) g_{200}^*(\vec{k}+\vec{k}_2-\vec{k}')I$$

where

$$(9) \qquad I = \int \frac{d\vec{r}}{r}\, e^{i\vec{k}_1'\cdot\vec{r}}\, H_{\vec{k}_1}(\vec{r}).$$

Referring to Appendix A, we have

$$I = \frac{4\pi i N(k')}{|2\vec{k}'+\vec{k}|^2}\left\{\frac{(\vec{k}-\vec{k}')\cdot(\vec{k}+2\vec{k}')}{(\vec{k}+2\vec{k}')^2}\right\}^{i/2a_o k'} .$$

Thus

$$(\vec{k}',200|R_{ex}|\vec{k},100) = \frac{4\pi e^2 N(\vec{k}')}{(\vec{k}+2\vec{k}')^2} \left\{ \frac{(\vec{k}-\vec{k}')\cdot(\vec{k}+2\vec{k}')}{(\vec{k}+2\vec{k}')^2} \right\}^{i/2a_o k'} \int d\vec{k}_2 g_o(\vec{k}_2) g_n^*(-\vec{k}'+\vec{k}_2+\vec{k})$$

or

$$(10) \quad (\vec{k}',200|R_{ex}|\vec{k},100) = \frac{2^{19/2}\pi e^2 a_o^2 N(k')|k-k'|^2}{|2\vec{k}'+\vec{k}|^2 \left\{9+4a_o^2|\vec{k}-\vec{k}'|^2\right\}^3} \left\{ \frac{(\vec{k}-\vec{k}')\cdot(\vec{k}+2\vec{k}')}{(\vec{k}+2k')^2} \right\}^{i/2a_o k'} .$$

C. Scattering cross sections:

The scattering cross section is given by

$$(11) \quad \sigma = (\frac{m}{\hbar^2})^2 \frac{k'}{k} \left\{ \frac{1}{4}|f+g|^2 + \frac{3}{4}|f-g|^2 \right\}$$

where f and g are the direct and exchange amplitudes. This can also be written in the form

$$(12) \quad \sigma = (\frac{m}{\hbar^2})^2 \frac{k'}{k} \left\{ |f|^2 + |g|^2 - \mathrm{Re} f g^* \right\} .$$

Substituting the values of f and g from (7) and (10) leads to

$$(13) \quad \sigma_{100\text{->}200} = \frac{2^{17}\pi e^{-\pi/k'}}{kk' \sinh \frac{\pi}{k'} \left[9+4|\vec{k}-\vec{k}'|^2\right]^6} \left\{ 1 + \frac{(\vec{k}-\vec{k}')^4}{(\vec{k}+2\vec{k}')^4} + \frac{(\vec{k}-\vec{k}')^2}{(\vec{k}+2\vec{k}')^2} \cos\left[\frac{1}{2k'} \log \frac{|\vec{k}+2\vec{k}'|^2}{|\vec{k}-\vec{k}'|^2}\right] \right\}.$$

The total cross section is

$$(14) \quad \Sigma_{100\text{->}200} = 2\pi \int_0^{\pi} \sigma_{100\text{->}200} \sin \theta d\theta.$$

This integral was computed numerically and led to the curve given in Figure 2. Comparison with the experimental results of Lichten[15] shows that the maximum we obtain is of the same order of magnitude but occurs at a higher energy. Lichten's maximum occurs at 11.7 e.v.

6. 1S-2P transition

A. Direct scattering

The main difference between the calculation for the 2P state and the 2S state lies in the evaluation of the integral

$$(1) \qquad I = \int d\vec{k}_2 g_o(\vec{k}_2) g_n^*(\vec{k}+\vec{k}_2-\vec{k}')$$

since the final state is not the same. This integral leads to

$$(2) \qquad I = i \frac{(3)2^{13/2}|\vec{k}-\vec{k}'|}{\left[9+4a_o^2|\vec{k}-\vec{k}'|^2\right]^3} .$$

This leads to

$$(3) \qquad (\vec{k}',210|R_d|\vec{k},100) = - \frac{2^{17/2}3i\pi e^2 a_o N(k')}{|\vec{k}-\vec{k}'|\left[9+4a_o^2|\vec{k}-\vec{k}'|^2\right]^3} \left\{ \frac{(\vec{k}-\vec{k}')\cdot(\vec{k}+2\vec{k}')}{(\vec{k}-\vec{k}')^2} \right\}^{i/2a_o k'} .$$

B. Exchange scattered amplitude

Again, the difference between the 2S and 2P lies in the momentum integral (1). Hence the exchange scattered amplitude is

$$(4) \qquad (\vec{k}',210|R_{ex}|\vec{k},100) = \frac{2^{17/2}\pi e^2 a_o N(k')|\vec{k}-\vec{k}'|}{|\vec{k}+2\vec{k}'|^2\left\{9+4a_o^2|\vec{k}-\vec{k}'|^2\right\}^3} \left[\frac{(\vec{k}-\vec{k}')\cdot(\vec{k}+2\vec{k}')}{|\vec{k}+2\vec{k}'|^2} \right]^{i/2a_o k'} .$$

C. Scattering cross section

The scattering cross section is obtained from equation (5.12) combined with (3) and (4). This yields

$$(5) \qquad \sigma_{100->200} = \frac{9x2^{16}\pi e^{-\pi/k'}}{kk'|\vec{k}-\vec{k}'|^2 \sinh\frac{\pi}{k'} \left[9+4|\vec{k}-\vec{k}'|^2\right]^6} \left\{ 1 + \frac{(\vec{k}-\vec{k}')^4}{(2\vec{k}'+k)^4} + \frac{(\vec{k}-\vec{k}')^2}{(2\vec{k}'+k)^2} \cos\left(\frac{1}{2k'} \log \frac{(\vec{k}+2\vec{k}')^2}{(\vec{k}-\vec{k}')^2} \right) \right\}.$$

The total cross section would then be

(6) $$\sum_{100\to 210} = 2\pi \int_0^{\pi} \sigma_{100\to 210} \sin \theta d\theta \ .$$

This integral was computed numerically and led to the curve given in Figure 3. Also included in this figure are the first Born approximation calculation[7], the second Born approximation[5] and Fite's experimental result[16]. Although the maximum in our curve is shifted toward the higher energies, it seems to us that it is a much better result than either of the approximations and simpler to calculate.

7. Discussion

The cross section for ionization and excitation to the 2S and 2P states of hydrogen have been calculated on the basis of the "Impulse Approximation." We note in Section 5 that, for the 2S-state, the agreement is not good although the magnitude is the same. For ionization and excitation to the 2P-state, the agreement is excellent and by far better than any other approximation method that is available. It therefore seems that it is possible to use the Impulse Approximation for calculating cross sections in the scattering of three or more body problems.

Appendix A

We evaluate here the integral given in equation (3.47)

(1) $$I = \int \frac{d\vec{r}}{r}\,\frac{e^{i\vec{q}\cdot\vec{r}}}{r}\,F(-in;1;ikr - i\vec{k}\cdot\vec{r}) \ .$$

We use the following integral representation for the confluent hypergeometric function[15]

(2) $$F(-in:1;ikr - i\vec{k}\cdot\vec{r}) = \frac{1}{2\pi i}\int_1^{(0+)} u^{-in-1}(u-1)^{in} e^{ikru - i\vec{k}\cdot\vec{r}u} du \ .$$

Substitution of (2) into (1) yields

(3) $$I = \frac{1}{2\pi i}\int_1^{(0+)} du\ u^{-in-1}(u-1)^{in} I(u)$$

where

(4) $$I(u) = \int \frac{d\vec{r}}{r}\exp\left[i\vec{q}\cdot\vec{r} + ikru - i\vec{k}\cdot\vec{r}u\right] \ .$$

I(u) is a standard integral that can be carried through to yield

(5) $$\begin{aligned} I(u) &= \frac{4\pi}{q^2 - 2\vec{q}\cdot\vec{k}u} \\ &= -\frac{2\pi}{(\vec{q}\cdot\vec{k})(u-u_o)} \end{aligned}$$

with $u_o = q^2/2\vec{q}\cdot\vec{k}$.

Thus

(6) $$I = \frac{i}{\vec{q}\cdot\vec{k}}\int_1^{(0+)} u^{-in-1}(u-1)^{in}(u-u_o)^{-1} du \ .$$

The contour for the representation of the hypergeometric function is given in Figure 1. Examination of the integrand in (6) shows that we have branch points at 0 and 1 and a simple pole at u_o. Thus we must deform the contour in such a way as to be able to include the pole u_o and not the branch points. This is accomplished by the contour given in Figure 2[13]. This contour is now clockwise. To compensate for the negative sign thus introduced, we put a negative sign in front of the integrand. Then applying Cauchy's theorem we get:

$$I = - \frac{2\pi}{\vec{q}\cdot\vec{h}} \frac{1}{u_o} \left(\frac{u_o - 1}{u_o}\right)^{in},$$

and since

$$u_o = \frac{q^2}{2\vec{q}\cdot\vec{h}},$$

we get

$$I = - \frac{4\pi}{q^2} \left[\frac{q^2 - 2\vec{q}\cdot\vec{h}}{q^2} \right]^{in} \qquad (7)$$

which is the integral given in the text.

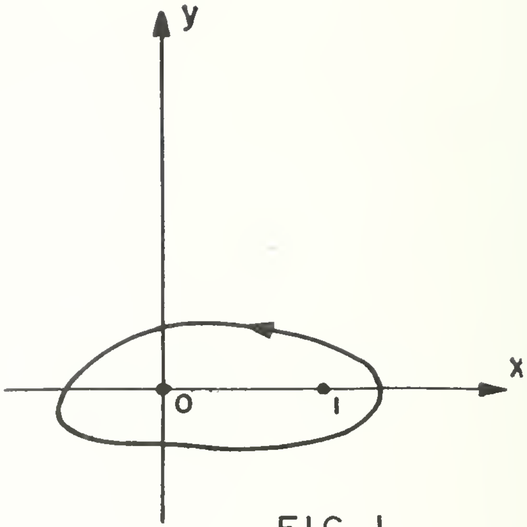


FIG. 1

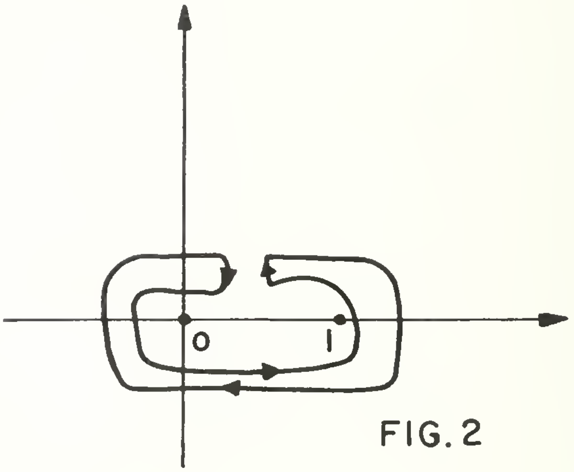


FIG. 2

Appendix B

We evaluate the integral occuring in the total ionization cross section. Dividing σ_t as given by equation (4.8) and putting h=m=e=1, we have

$$(1) \qquad \sigma_t = \frac{2^8\pi^3}{k_1} \iint d\vec{k}_1' d\vec{k}_2' \, \frac{e^{-\pi/|2\vec{k}_1-\vec{k}_1'-\vec{k}_2'|}}{\sinh(\pi/|2\vec{k}_1-\vec{k}_1'-\vec{k}_2'|)} \, \frac{\delta\left\{\frac{1}{2}\left[k_1'^2+k_2'^2-k_1^2+1\right]\right\}}{|\vec{k}_1-\vec{k}_1'|^4 \, |2\vec{k}_1-\vec{k}_1'-\vec{k}_2'|^2 \left[1+|\vec{k}_1-\vec{k}_1'-\vec{k}_2'|^2\right]^4}$$

The cross section is expressed now in units of πa_o^2; the unit of length is the Bohr radius, and the unit of energy twice the ionization energy of hydrogen.

Let

$$\vec{k} = \vec{k}_1 - \vec{k}_1'$$
$$\vec{k}' = \vec{k}_1 - \vec{k}_2' \quad .$$

Then:

$$(2) \qquad \sigma_t = \frac{2^8\pi^3}{k_1} \iint d\vec{k}d\vec{k}' \, \frac{e^{-\pi/|\vec{k}+\vec{k}'|}}{\sinh \pi/|\vec{k}+\vec{k}'|} \, \frac{\delta\left(\frac{1}{2}\left(k_1^2+k^2+k'^2+1-2\vec{k}_1\cdot(\vec{k}+\vec{k}')\right)\right)}{k^4(\vec{k}+\vec{k}')^2 \left\{1+|\vec{k}_1-\vec{k}-\vec{k}'|^2\right\}^4} \quad .$$

Let

$$(3) \qquad \left.\begin{array}{l} \vec{k}-\vec{k}' = \vec{\lambda} \\ \vec{k}+\vec{k}' = \vec{K} \end{array}\right\} \;->\; \left\{\begin{array}{l} \vec{k} = 1/2(\vec{K}+\vec{\lambda}) \\ \vec{k}' = 1/2(\vec{K}-\vec{\lambda}) \end{array}\right.$$

then

$$k^2+k'^2 = \frac{1}{2}(K^2+\lambda^2)$$
$$d\vec{k}d\vec{k}' = \frac{1}{2^3} d\vec{\lambda} d\vec{K}$$

Thus

$$(4) \qquad \sigma_t = - \frac{2^9\pi^3}{k_1} \int d\vec{K} \, \frac{e^{-\pi/K}}{\sinh \pi/K} \, \frac{1}{K^2\left[1+|\vec{k}_1-\vec{K}|^2\right]^4} \, I(\vec{K}) \quad .$$

with

$$(5) \qquad I(\vec{K}) = \int d\vec{\lambda} \, \frac{\delta\left\{\frac{1}{4}\left[\lambda^2-(4\vec{k}_1\cdot\vec{K}-2k_1^2-K^2-2)\right]\right\}}{(\vec{K}+\vec{\lambda})^4} \quad .$$

The angular integration can be carried through easily leading to

(6) $$I(\vec{K}) = 4\pi \int_{-\infty}^{\infty} \lambda^2 \, \frac{\delta\left\{\frac{1}{4}(\lambda^2 - [4\vec{k}_1\cdot\vec{K} - 2k_1^2 - K^2 - 2])\right\}}{(K^2-\lambda^2)^2} \, d\lambda \; .$$

The limits, due to the δ-function, will run over the entire space. Now let

$$a^2 = 4\vec{k}_1\cdot\vec{K} - 2k_1^2 - K^2 - 2 \; .$$

Then

$$\begin{aligned} \delta\left(\tfrac{1}{4}\,(\lambda^2 - a^2)\right) &= 4\delta(\lambda^2 - a^2) \\ &= \frac{2}{a}\Big(\delta(\lambda + a) + \delta(\lambda - a)\Big) \; . \end{aligned}$$

Substituting into (6) and carrying out the integration yields:

(7) $$I(\vec{K}) = \frac{4\left\{4\vec{k}_1\cdot\vec{K} - 2k_1^2 - K^2 - 2\right\}^{1/2}}{\left|1 + |\vec{k}_1 - \vec{K}|^2\right|^2} \; .$$

Then

$$\begin{aligned} \sigma_t &= -\frac{2^{11}\pi^3}{k_1}\int \frac{d\vec{K}}{K^2}\, \frac{e^{-\pi/K}}{\sinh \pi/K}\, \frac{(4\vec{k}_1\cdot\vec{K} - 2k_1^2 - K^2 - 2)^{1/2}}{\left\{1 + |\vec{k}_1 - \vec{K}|^2\right\}^6} \\ &= -\frac{2^{12}\pi^3}{k_1}\int dK\, \frac{e^{-\pi/K}}{\sinh \pi/K} \int_{-1}^{1} \frac{(-2k_1^2 - K^2 - 2 + 4k_1Kx)^{1/2}}{\left[1 + k_1^2 + K^2 - 2k_1Kx\right]^6}\, dx \; . \end{aligned}$$

Carrying through the second integral, we obtain

$$\sigma_t = \frac{2^{15}\pi^3}{15k_1^2}\,\sigma_1 + \frac{2^{12}\pi^3}{5k_1^2}\,\sigma_2 + \frac{2^{11}\pi^3}{15k_1^2}\,\sigma_3 + \frac{7\text{x}2^9\pi^3}{3k_1^2}\,\sigma_4 + \frac{7\text{x}2^9\pi^3}{k_1^2}\,\sigma_5 - \frac{7\text{x}2^9\pi^3}{k_1^2}\,\sigma_6$$

where

$$\sigma_1 = \int \left\{ \frac{\sqrt{-4k_1K + 2k_1^2 + K^2 + 2}}{\left[1 + (k_1 - K)^2\right]^5} - \frac{\sqrt{4k_1K + 2k_1^2 + K^2 + 2}}{\left[1 + (k_1 - K)^2\right]^5} \right\} \frac{dK}{K}\, \frac{e^{-\pi/K}}{\sinh \pi/K}$$

$$\sigma_2 = \int \left\{ \frac{\sqrt{-4k_1K + K^2 + 2k_1^2 + 2}}{\left[1 + (k_1 - K)^2\right]^4} - \frac{\sqrt{4k_1K + 2k_1^2 + K^2 + 2}}{\left[1 + (k_1 - K)^2\right]^4} \right\} \frac{e^{-\pi/K}}{\sinh \pi/K}\, \frac{dK}{K^3}$$

$$\sigma_3 = \int \left\{ \frac{\sqrt{-4k_1K+K^2+2k_1^2+2}}{\left[1+(k_1-K)^2\right]^3} - \frac{\sqrt{4k_1K+2k_1^2+K^2+2}}{\left[1+(k_1-K)^2\right]^3} \right\} \frac{e^{-\pi/K}}{\sinh \pi/K} \frac{dK}{k^5}$$

$$\sigma_4 = \int \left\{ \frac{\sqrt{-4k_1K+K^2+2k_1^2+2}}{\left[1+(k_1-K)^2\right]^2} - \frac{\sqrt{4k_1K+2k_1^2+K^2+2}}{\left[1+(k_1-K)^2\right]^2} \right\} \frac{e^{-\pi/K}}{\sinh \pi/K} \frac{dK}{K^7}$$

$$\sigma_5 = \int \left\{ \frac{\sqrt{-4k_1K+K^2+2k_1^2+2}}{\left[1+(k_1-K)^2\right]} - \frac{\sqrt{4k_1K+2k_1^2+k^2+2}}{\left[1+(k_1-K)^2\right]} \right\} \frac{e^{-\pi/K}}{\sinh \pi/K} \frac{dK}{K^9}$$

$$\sigma_6 = \int \left\{ \tanh^{-1} \frac{K\sqrt{+4k_1K+2k_1^2+K^2+2}}{2+2k_1^2+K^2} + - \tanh^{-1} \frac{K\sqrt{-4k_1K+2k_1^2+K^2+2}}{2+2k_1^2+K^2} \right\} \frac{e^{-\pi/K}}{\sinh \pi/K} \frac{dK}{K^{10}}$$

The limits of integration are

$$K_{min} = 2k_1 - \sqrt{k_1^2-1}$$

$$K_{max} = 2k_1 + \sqrt{k_1^2+1} \quad .$$

This follows from the discussion in Section 4.

Appendix C

We evaluate here the integral appearing in Section 5, namely equation 6.

(1) $$I_n = \int d\vec{r}\, \Phi_n^*(\vec{r}) e^{i(\vec{k}-\vec{k}')\cdot\vec{r}}\, \Phi_o(\vec{r}) .$$

Now

(2a) $$\Phi_o(\vec{r}) = (4\pi a_o^3)^{-1/2}\, e^{-r/a_o} .$$

For final states, we have

(2b) 2S: $$\Phi_{200}(\vec{r}) = (2^5\pi a_o^3)^{-1/2}\,(2-r/a_o)e^{-r/2a_o}$$

(2c) 2P: $$\Phi_{210}(\vec{r}) = \left[2^5\pi a_o^3\right]^{-1/2} \frac{r}{a_o}\, e^{-r/2a_o} \cos\theta .$$

1. 2S-state

(3) $$I_{200} = \frac{1}{2^{7/2} a_o^3 \pi} \int d\vec{r}\, e^{i(\vec{k}-\vec{k}')\cdot\vec{r}}\,(2-r/a_o)e^{-3r/2a_o} .$$

Let

$$x = \frac{r}{a_o} \qquad \text{and} \qquad \vec{K} = a_o(\vec{k}-\vec{k}')$$

then

$$I_{200} = \frac{1}{2^{7/2}\pi} \int_0^\infty x^2 dx e^{-3x/2}\,(2-x) \int_0^\pi e^{iKx\cos\theta} \sin\theta d\theta \int_0^{2\pi} d\phi$$

(4) $$= \frac{1}{2^{5/2} iK} \int_0^\infty dx\, x(2-x)e^{-3x/2}(e^{iKx}-e^{-iKx})$$

$$= \frac{1}{2^{5/2} iK} \left\{ 2(\lambda_1 - \lambda_1^*) - (\lambda_2 - \lambda_2^*) \right\}$$

where

(5a) $$\lambda_1 = \int_0^\infty x dx e^{-(3/2 - iK)x}$$

(5b) $$\lambda_2 = \int_0^\infty x^2 dx e^{-(3/2 - iK)x}$$

These are standard integrals and yield

$$(6a)\qquad \lambda_1 = \frac{4}{(3-2iK)^2}$$

$$(6b)\qquad \lambda_2 = \frac{16}{(3-2iK)^3} \; .$$

Hence

$$(7a)\qquad \lambda_1 - \lambda_1^* = \frac{3\cdot 2^5 iK}{(9+4K^2)^2}$$

$$(7b)\qquad \lambda_2 - \lambda_2^* = \frac{2^6 iK(27-4K^2)}{(9+4K^2)^3} \; .$$

Substituting into (4), we get

$$(8)\qquad I_{200} = \frac{2^{15/2}K^2}{(9+4K^2)^3} = \frac{2^{15/2}|\vec{k}-\vec{k}'|^2}{\left\{9+4|\vec{k}-\vec{k}'|^2\right\}^3} \; .$$

2. 2P-state

$$(9)\qquad I_{210} = \frac{1}{2^{7/2}\pi a_o^4}\int r d\vec{r}\; e^{+i(\vec{k}-\vec{k}')\cdot\vec{r}}\; e^{-3r/2a_o} \cos\theta \; .$$

The same substitution is carried out for $\vec{r}$ and $\vec{k}-\vec{k}'$ as for I_{200}, yielding

$$I_{210} = \frac{1}{2^{5/2}}\int_0^\infty x^3 dx e^{-3x/2}\int_0^\pi e^{iKx\cos\theta}\cos\theta\sin\theta d\theta \; .$$

These are simple integrals and can be carried through to yield

$$(10)\qquad I_{210} = \frac{3i\; 2^{13/2}|\vec{k}-\vec{k}'|}{\left\{9+4|\vec{k}-\vec{k}'|^2\right\}^3} \; .$$

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